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H. L. Grubin and T. R. Govindan

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This report summarizes work performed under Contract DAAL03-90-C-0005. The study represents the first comprehensive effort to assess through (1) numerical simulations of the equation of motion of the density matrix, and (2) approximate analytical procedures involving an expansion of the Liouville potential, the multiplicative constant associated with the quantum potential as used in quantum hydrodynamic transport. It was found that when quantum effects are 'corrections' to classical calculations, as in $N^+N^-N^+$ structures the factor '1/3' is a satisfactory multiplicative constant. When the quantum potential is no longer a correction, as in the case of double barrier diodes, the multiplicative constant is no longer 'constant' but is position dependent and less than unity.

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INTRODUCTION

The development of crystal growth techniques has made it possible to fabricate devices with very small dimensions and sharp interfaces. Consequently, a variety of device concepts based upon small dimensions with sharp interfaces has emerged. These include such high speed devices as the HEMT, HBT, quantum resonant tunneling devices, quantum wire structures and quantum dots. The structure and operation of these devices is based upon a perceived physical picture, often based upon results of quantum transport theory.

While all devices are governed and sometimes limited by quantum mechanical properties, many devices do not require quantum mechanics for an understanding of their basic operation, but do need quantum mechanics to provide key electrical properties. For example, heterostructure bipolar transistors sustain low levels of current at low bias levels; these currents are dominantly tunneling currents. Thermionic contributions to current occur at high bias levels. Until recently, the drift and diffusion equations as well as the moments of the Boltzmann transport equation did not include a description of tunneling currents in any way other than through ad hoc arguments. Tunneling requires quantum mechanical contributions.

The recent advance in the description of transport in devices with quantum contributions is due to the discussion of Ancona and Iafrate (1989), who demonstrated that the quantum corrections to multi-particle transport, first discussed by Wigner (1932), could be incorporated in the drift and diffusion equations by adding to the classical potential a term proportional to a quantum mechanical based potential:

(1) $\qquad Q = -(\hbar^2/2m)[(\rho)^{\frac{1}{2}}{}_{xx}]/(\rho)^{\frac{1}{2}}$

where the subscripts denote derivatives. Within the framework of the drift and diffusion equation the 'Q' term modifies the particle current as follows:

(2) $\qquad j(x,t) = n\mu k_b T[(V + aQ)/k_b T + \ell n(n)]_x$

The proportionality constant 'a' was evaluated [Ancona and Iafrate (1989)] in the high temperature limit from the equation of motion of the Wigner function and was found to be equal to 1/3. The factor '1/3' is a serious issue, in that intuitively, as well as through arguments associated with the single particle Schrodinger equation, it would be anticipated that the constant 'a' would be unity.

The problem addressed in the last paragraph, namely the origin of the factor a = 1/3, as well as the **procedures under which quantum contributions to the balance equations are obtained** formed the basis of the study under Contract DAAL03-90-C-0005. This was

complemented by numerical simulations, using 'characteristic' algorithms to examine the extent to which the quantum corrected results are relevant.

The means by which the problem is addressed is through an expansion of the equation of motion of the Wigner function, and an expansion of the equation of motion of the density matrix. The discussion of the Wigner function is in the form of a review, in that a comprehensive treatment appears in Grubin and Kreskovsky (1989). The work on the density matrix is new.

QUANTUM CORRECTED EQUATIONS OF MOTION FOR THE WIGNER FUNCTION AND THE DENSITY MATRIX

The Wigner Equation of Motion: The analysis under this study was restricted to one space and one momentum direction and includes Fokker-Planck scattering. The equation of motion of the Wigner function with Fokker-Planck dissipation as discussed by Stroscio (1986) is:

$$(3) \quad f_t + (p/m)f_x + (1/i\hbar)(1/2\pi\hbar)_{-\infty}\int^{+\infty}dp'_{-\infty}\int^{+\infty}dx'f(p',x)[V(x,x',t)]\exp[i(p-p')x'/\hbar]$$

$$= 2\gamma[pf]_p + Df_{pp}$$

where:

$$(4) \quad V(x,x',t) = [V(x+x'/2,t)-V(x-x'/2,t)]$$

The potential energy $V(x,x',t)$ is referred to below as the Liouville potential. As discussed by Frensley (1990) the first term of the Fokker-Planck dissipation corresponds to a frictional damping term, the second corresponds to thermal fluctuations. This will be discussed in more detail below.

It is direct, but nontrivial to demonstrate that the integral in equation (3) reduces in the classical case to $V_x f_p$; thus equation (3) reduces to the Boltzmann transport equation with Fokker-Planck dissipation:

$$(5) \quad f_t + (p/m)f_x - V_x f_p = 2\gamma[pf]_p + Df_{pp}$$

To second order in $\hbar$, the Wigner equation of motion, or equivalently, the quantum corrected Boltzmann equation is:

$$(6) \quad f_t + (p/m)f_x - V_x f_p + (\hbar^2/24)V_{xxx}f_{ppp} = 2\gamma[pf]_p + Df_{pp}$$

The left hand side of equation (6) has been discussed in detail by Ancona and Iafrate (1989) and Grubin and Kreskovsky (1989).

The Equation of Motion of the Density Matrix: This equation has been discussed in the context of quantum structures by Frensley (1990). While the equation of motion is a fundamental equation, it is equivalent to and can be obtained directly from the Wigner equation of motion. In the latter case multiply equation (3) by $dp[\exp[i2\zeta p/\hbar]]$ and integrate over p. For this integration p varies from $-\infty$ to $+\infty$, and it is assumed that the Wigner function and all necessary derivatives with respect to momentum vanish as $p\Rightarrow\pm\infty$. Identifying the density matrix through the Weyl transformation:

$$(7) \quad \rho(x+\zeta,x-\zeta) = [1/(2\pi\hbar)]_{-\infty}\int^{\infty}dpf_W(p,x)\exp[2ip\zeta/\hbar]$$

the transformed equation becomes the density matrix in the coordinate representation:

$$(8) \qquad \rho_t + (\hbar/2mi)\rho_{x\varsigma} - (1/i\hbar)[V(x+\varsigma,t)-V(x\varsigma,t)]\rho + 2\gamma\varsigma\rho_\varsigma + [4D\varsigma^2/\hbar^2]\rho = 0$$

An expansion of the Liouville potential about the point x yields:

$$(9) \qquad \rho_t + (\hbar/2mi)\rho_{x\varsigma} - (1/i\hbar)[2\varsigma V_x + (\varsigma^3/3)V_{xxx}]\rho + 2\gamma\varsigma\rho_\varsigma + [4D\varsigma^2/\hbar^2]\rho = 0$$

which is the transformed equivalent of equation (6).

Retaining only the terms that are linear in ς yields the transformed equivalent to the classical Boltzmann equation. As will be seen the presence of the factor '1/3' in equation (9) is the key ingredient in obtaining the multiplicative factor in the quantum potential. It is emphasized that quantum corrections to $O(\hbar^2)$ are contained in the term $[(\varsigma^3/3)V_{xxx}]\rho$.

Equations (6) and (9) are the relevant equations for the analytical part of this study. Equations (3) and (8) are, however, the ones to deal with in a fundamental approach to quantum transport. Results with equation (8) are introduced later into the discussion.

THE APPROXIMATE EQUILIBRIUM DISTRIBUTION FUNCTION

In the absence of dissipation the approximate Wigner distribution function to second order in $\hbar$ is Wigner (1932):

$$(10) \qquad f_w = \exp{-\beta}[p^2/2m + U(x)]\{1-(\lambda^2\beta/4)[(V_{xx}-\beta V_x^2/3)-\beta(p^2/3m)V_{xx}]\}$$

Where $\lambda^2 = \hbar^2\beta/2m$, and $\beta = 1/(k_bT)$. The equivalent approximate density matrix solution to order $O(\hbar^2)$ is:

$$(11) \qquad \rho(x+\varsigma,x-\varsigma) = N\exp{-[\varsigma^2/\lambda^2 + \beta V]}\{1-(\lambda^2\beta/6)(1+\varsigma^2/\lambda^2)V_{xx}+\lambda^2\beta^2 V_x^2/12\}$$

where,

$$(12) \qquad N = 2(m/2\pi\beta\hbar^2)^{1/2}.$$

Note: First, the classical density matrix equivalent to the Boltzmann distribution is:

$$(13) \qquad \rho(x+\varsigma,x-\varsigma) = N\exp{-[\varsigma^2/\lambda^2 + \beta V]};$$

Second, the brackets $\{\bullet\bullet\bullet\}$ contains quantum corrections to the density matrix. Third, the approximate density matrix is real, indicating that the current is zero. Fourth, the diagonal components of the approximate density matrix, which are obtained for $\varsigma = 0$, are equal to:

$$(14) \qquad \rho(x,x) = N[\exp{-\beta V}][1-(\lambda^2\beta/6)(V_{xx}-\beta V_x^2/2)]$$

This result also emerges from an integration of the Wigner function over all values of momentum (Ancona and Iafrate (1989).

The significance of equation (14) for device applications is that it describes the way in which quantum corrections alter the built-in potential. For example, when it is recalled that, classically, the potential and carrier density are related through the expression:

$$(15) \qquad \rho = N\exp{-\beta V}$$

and therefore that $\beta V_x = -\rho_x/\rho$; then through incorporation of the quantum potential (equation (1)), it is straightforward to show that $Q = (\hbar^2/4m)\beta[V_{xx}-\beta V_x^2/2]$, and that:

(16) $\rho = N[\exp{-\beta V}][1-(\beta Q/3)]$

Several points are clear: First there may be an alteration of the built-in potential arising from gradients in the carrier density; second, the factor of '3' that appears in equation (16) is seen to be a consequence of the truncation of the Taylor expansion of the potential in both the density matrix and Wigner equations.

Quantum Corrected Energy Density Matrix: There is a characteristic energy associated with the equilibrium system obtained from both the Wigner function and the density matrix. To obtain it from the density matrix we define an energy density matrix through a Weyl-like transformation:

(17) $E(x+\zeta,x-\zeta) = [1/(2\pi\hbar)]_{-\infty}\int^{\infty}dp(p^2/2m)f_W(p,x)\exp[2ip\zeta/\hbar]$

Note: for $\zeta = 0$, the above reduces to mean kinetic energy of the system. It is direct to demonstrate that

(18) $E(x+\zeta,x-\zeta) = -(\hbar^2/8m)\rho_{\zeta\zeta}$

The expectation value of the energy is the diagonal component of the energy density matrix, and yields:

(19) $E(x,x) = [\rho k_b T/2[[1-(\lambda^2/6)(\ell n\rho)_{xx}]$

$= [k_b T/2 + w_q]\rho$

The term w_q was first introduced by Wollard et al (1990). Equation (19) is valid only to second order in $\hbar$. Thus the density multiplying the term '$(\ell n\rho)_{xx}$' is strictly only the classical density. The significance of equation (11) is that there is a change in energy due to the gradients of carrier density, as first predicted by Wigner (1932).

THE APPROXIMATE NONEQUILIBRIUM DENSITY MATRIX

Classical moment balance equations are often obtained through representing the nonequilibrium state by a displaced Maxwellian, $\exp{-[\beta\{(p-p_d)^2/2m + V\}]}$ where, e.g., p_d, the density and a particle temperature, are to be determined. The Weyl transformation indicates that a displaced Maxwellian yields a density matrix with the following modification:

(20) $\rho(x+\zeta,x-\zeta) \Rightarrow \rho(x+\zeta,x-\zeta)\exp{-[2ip_d\zeta/\hbar]}$

Thus the classical density matrix corresponding to the displaced Maxwellian is (21)
$\rho(x+\zeta,x-\zeta) = N\exp{-[\zeta^2/\lambda^2 + \beta V + 2ip_d\zeta/\hbar]}$

Note that the density matrix contains an imaginary part, as required for a finite current. The nonequilibrium quantum-corrected density matrix is given by a modification of equation (11):

(22) $\rho(x+\zeta,x-\zeta) = N\exp\text{-}[\zeta^2/\lambda^2 + \beta V + 2ip_d\zeta/\hbar]$

$$\{1\text{-}(\lambda^2\beta/6)(1+\zeta^2/\lambda^2)V_{xx} + \lambda^2\beta^2 V_x{}^2/12\}$$

<u>Quantum Corrected Current (velocity flux) Density Matrix</u>: Since the density matrix contains imaginary components we are interested in the expectation values of the current flux density. To obtain this we define a current density matrix as:

(23) $j(x+\zeta,x-\zeta) = [1/(2\pi\hbar)]_{-\infty}\int^{\infty} dp(p/m)f_w(p,x)\exp[2ip\zeta/\hbar]$

Note: for $\zeta = 0$, the above reduces to mean velocity flux of the system. It is direct to show that:

(24) $j(x+\zeta,x-\zeta) = (\hbar/(2mi))\rho_\zeta$

The expectation value of current is the diagonal component:

(25) $j(x,x) = (p_d/m)\rho$

The quantum corrections to the current are obtained from the quantum corrections to the density. Note that the form of the current density along the diagonal is the same for classical transport as it is for quantum corrected transport. Thus of relevance are the equations defining p_d, density and temperature. To establish these we reconsider the equation of motion of the density matrix taking successive derivatives.

THE APPROXIMATE NONEQUILIBRIUM BALANCE EQUATIONS AS OBTAINED FROM THE EQUATION OF MOTION OF THE DENSITY MATRIX

<u>Particle Balance</u>: The first balance equation is obtained by rewriting the equation of motion of the density matrix and then dealing only with the diagonal component. Thus there is reduced content. Using the definition of velocity flux, equation (9) becomes:

(26) $\rho(x+\zeta,x-\zeta)]_t + [j(x+\zeta,x-\zeta)]_x - (1/i\hbar)[2\zeta V_x + \zeta^3 V_{xxx}/3]\rho(x+\zeta,x-\zeta)$

$$+2\gamma\zeta[\rho(x+\zeta,x-\zeta)]_\zeta + [4D\zeta^2/\hbar^2]\rho(x+\zeta,x-\zeta) = 0$$

<u>The first balance equation</u> is obtained from the diagonal component of equation (24):

(27) $[\rho]_t + [\rho p_d/m]_x = 0$

which is the equation of continuity.

<u>Momentum Balance</u>: To determine the next governing equation to second order in $\hbar$ we take derivatives of equation (2) with respect to 'ζ', multiply by $\hbar/2i$, and obtain:

(28) $[p(x+\zeta,x-\zeta)]_t + 2[E(x+\zeta,x-\zeta)]_x + (1/2)[2V_x + \zeta^2 V_{xxx}]\rho(x+\zeta,x-\zeta)$

$$-(1/i\hbar)[2\zeta V_x + \zeta^3 V_{xxx}/3]p(x+\zeta,x-\zeta)$$

$$+2\gamma p(x+\zeta,x-\zeta) - i[4D\zeta/\hbar]\rho(x+\zeta,x-\zeta)$$

$$-i\hbar\gamma\zeta[\rho(x+\zeta,x-\zeta)]_{\zeta\zeta} + [4D\zeta^2/\hbar^2][p(x+\zeta,x-\zeta)] = 0$$

where $p(x+\zeta,x-\zeta) = j(x+\zeta,x-\zeta)m$. The diagonal component of energy under finite current conditions is required for the second balance equation. It is:

(29) $\quad E(x,x) = [p_d^2/2m + (k_bT/2)(1-(\lambda^2/6)(\ell n\rho)_{xx}]\rho$

With the diagonal components of energy given by equation (29), identifying a relaxation time $\tau = 2/\gamma$, the second balance equation is obtained from the diagonal components of equation (29):

(30) $\quad (\rho p_d)_t + (\rho p_d^2/m)_x + (\rho kT)_x + \rho(Q/3)_x + \rho V_x + \rho p/\tau = 0$

where we recognize that $[(\ell n\rho)_{xx}\rho]_x = -4m\rho Q_x/\hbar^2$. The above equation differs from its classical analog through the presence of the quantum potential. The form of the scattering term in the above equation also confirms Frensley's (1990) statement of the first part of the Fokker-Planck scattering as a frictional term.

Energy Balance: If we regard the quantum corrected density matrix as a distribution function with three undetermined parameters, the third being the temperature, then a third equation is needed to complete the system of equations. This third equation is obtained in a manner similar that of equation (28), namely by taking a second derivative of the density matrix equation of motion, with respect to ζ. We are only interested in the diagonal components of this equation, which with the energy given by equation (18), are:

(31) $\quad E_t + (1/(2m^2))P^3{}_x + jV_x = (E_t)_{coll}$

where P^3 is the diagonal component of the third moment of the off-diagonal element:

(32) $\quad [1/(2\pi\hbar)]_{-\infty}\int^{\infty}dp(p^3)f_w(p,x)exp[2ip\zeta/\hbar] = (\hbar/2i)^3\rho_{\zeta\zeta\zeta}$

Using equation (21) for the density matrix, equation (32) becomes:

(33) $\quad E_t + \{(p_d/m)[E + (\rho/\beta)(1-[\lambda^2/6](\ell n\rho)_{xx})]\}_x + (\rho p_d/m)U_x + 2E/\tau + 8D\rho = 0$

where the energy in equation (33) is given by equation (29) (Note: the equilibrium value of P^3 is zero). The above equation can be rearranged to read:

(34) $\quad E_t + (p_dE/m)_x + (p_d\rho k_bT/m)_x + (\rho p_d/m)[Q/3 + V]_x$

$\quad\quad\quad -\rho(\lambda^2 k_bT/6)[(\ell n\rho)_{xx}](p_d/m)_x + 2E/\tau - 8D\rho = 0$

If we assume equilibrium values for D, namely $D = mk_bT/\tau$, equation (34) becomes:

(35) $\quad E_t + (p_dE/m)_x + (p_d\rho k_bT/m)_x + (\rho p_d/m)[Q/3 + V]_x$

$\quad\quad\quad -\rho(\lambda^2 k_bT/6)[(\ell n\rho)_{xx}](p_d/m)_x + (2/\tau)[E-k_bT/2]\rho = 0$

And the second part of the Fokker-Planck dissipation involves a relaxation to a non-zero thermal energy.

The equation of motion of the density matrix involves two NxN matrices (real and imaginary parts) where N represents the numbers of grid points along a linear dimension. The density matrix equation is the equation of interest. An approximate representation of the equation of motion of the density matrix is provided by the first three moments of the density matrix. These moments include the continuity equation, momentum balance, and

energy balance.

As in all moment equation representations, the form of the moment equation depends upon the primary equation, in this case equation (9), and the generic form of the distribution function, in this case equation (22). The most dramatic consequence of the approach, as expressed in the momentum balance equations, is the appearance of the quantum potential. The quantum potential with its associated factor of '1/3', the latter arising solely as a consequence of the expansion of the Liouville potential, permits a quantum mechanical "correction" description of classical transport and allows tunneling to be incorporated into the latter. This result was also the initial conclusion of Ancona and Iafrate (1990).

It is important to reiterate that one key result of the present study is that through the expansion of Liouville potential in the equation of motion of the density matrix the quantum corrections are the same as those obtained from the equation of motion of the Wigner distribution function. The origin of the factor of '1/3' is due solely to the expansion of the Liouville potential, and is not limited the high temperature limit discussed by Ancona and Iafrate (1989).

The energy balance equation is also driven by the quantum potential, but additionally there appears to be a contribution that may behave as a quantum correction to the pressure. This is the terms $\rho(\lambda^2 k_b T/6)[(\ell n\rho)_{xx}]$.

In addition to the quantum mechanical contributions, the moment equations include an incorporation of Fokker-Planck dissipation in the moment formulation, and twenty of the relative contribution of each of the two terms. A more general treatment is provided by Stroscio (1986).

The next question concerns the significance of the quantum potential.

SELF CONSISTENT NUMERICAL SOLUTIONS

This section contains a discussion of the **interpretation** of the distribution of charge within the quantum well and quantum barrier device and the values obtained thereof. The calculations involve solutions to the density matrix coupled to Poisson's equation:

$$(36) \qquad \partial/\partial x[\epsilon(x)\partial V/\partial x] = -e^2[\rho(x,x)-\rho_o(x)]$$

Classical N$^+$N$^-$N$^+$ Structures: Since most resonant tunnel structures are designed with the heterostructures placed within the interior of a low doped region, the first self-consistent problem discussed involves transport through a classic N$^+$N$^-$N$^+$ structure. The structure is 1200Å long with a nominal doping of 10^{18}/cm^3 and a centrally placed 250Å, 10^{15}/cm^3 region. The variation in background doping was over one grid point or 4Å.

There are a variety of questions to be addressed here; among them is the issue of whether there are any quantum contributions associated with an ostensibly classical structure. It is relevant, in this matter to recall one of the conclusions of a paper by Iafrate, Grubin and Ferry (1981), where it was argued that quantum corrections are important if the density sustained an approximate Gaussian distribution with a width at half maximum of approximately 80Å of less.

The equilibrium charge density and potential distribution as obtained from the complete equation of motion of the density matrix, equation (8) without dissipation, for the N$^+$N$^-$N$^+$ structure are shown in figures (1a) and (1b), respectively. The results appear classical. We also show the diagonal component of energy density of the system, figure (1c),

ar computed from equation (18) and the quantum potential, figure (1d), as computed from equation (1). For completeness we also show the two dimensional plot of the density matrix in figure 2.

Figures (1a) and (1b) display charge density and self-consistent potential distributions that are ostensibly classical. There is an increase in potential across the N^- region, which accompanies a decrease in charge density across this same region. From the point of view of quantum transport, we are also dealing with a tunneling problem, particularly with those carriers whose energy is below the potential barrier, which in this case has a height of approximately 45 mev. We note that the mean energy of the entering carriers is $k_b T/2 < 45$ mev.

Quantum transport permits tunneling, thereby increasing the numbers of particles in the N^- region over the classical value. Continuity of the wavefunction and its derivative through the barrier region (at the metallurgical interface the energy density is approximately $k_b T\rho/2$, and decreases into the N^- region) prevents the density from approaching it's classical value, and instead assumes a smaller value. This result which is a consequence of wave function continuity has been referred to by others as quantum "repulsion" (Kluksdahl et al (1989)). The "increased" value of density in the barrier region and "decreased" value of density in the classically accessible region are represented by equation (16) if the quantum is negative within the barrier region and positive within the region of the 'turning points' at the boundary of the metallurgical junction. The quantum potential as evaluated from equation (1) and depicted in figure 1d displays these qualitative features. Note that the quantum potential at the center of the structure is approximately 25% of the energy at the boundaries. For a very wide N^- region the density at the center region of the structure will be relatively constant and $Q \lesssim 0$, at the center.

For the calculation of figures 1 and 2, the density, potential and quantum potential are respectively

(37) $\rho_{cal}(v=0) = 1.847 \times 10^{17}/cm^3$

(38a) $V_{cal}(x=0) = 44.725$ mev

(38b) $Q_{cal}(x=0) = -3.0228$ mev

Calculations $\rho(x=0)$ from equation (16) with the potential energy and quantum potential given by equation 38 yield

(39) $\rho_{Eq.(38)}(x=0) = 1.832 \times 10^{17}/cm^3$

The energy density at the center of the structure as computed from the density matrix is

(40) $E_{cal}(x=0) = 2.3015$ mev/cm^3

The energy as computed from equation (19) is

(41) $E_{Eq.(19)}(x=0) = 2.286$ mev/cm^3

The hydrodynamic moment equations appear in the case of the simple $N^+N^-N^+$ to yield the same result as the density matrix for the charge distribution.

Double Barrier Diodes: The situation for double barrier diodes is quantitatively different than that of the $N^+N^-N^+$ structure. Here the quantum mechanics is not a correction to the classical solution. However, as in the $N^+N^-N^+$ structure, it is expected that outside of the double barrier that continuity of the wave function would again yield a density below that of the classical value. Thus the quantum potential would be positive in this region. Within the barrier quantum mechanical tunneling permits a greater number of carriers than those associated with the classical distribution; thus the quantum potential is negative. Within the quantum well continuity of the wavefunction results in a charge distribution that is below that obtained classically; and Q is negative. The variation of density, potential, energy and quantum potential are displayed in figures 3 and 4.

Figure 3a displays the density distribution which shows a small residual change in the quantum well and an insignificant amount of charge within the barriers. Potential energy is displayed in figure 3b, where we note that the low density in the quantum well region contributes to an elevation of the potential relative to the end points. The mean energy density is shown in figure 3c, and displays negligible values at the center of the structure. The quantum potential is displayed in figure 3d. For the calculations of figure 3, the density potential energy and quantum potential are respectively

(42) $\rho_{cal}(x=0) = 6.156 \times 10^{16}/cm^3$

(43a) $V_{cal}(x=0) = 15.479 \ mev$

(43b) $Q_{cal}(x=0) = 92.149 \ mev$

Calculating $\rho(x=0)$ from equation (16) within the potential energy and quantum potential given by equation (43) requires that the quantum potential be multiplied by a constant other than 1/3. For the present situation the constant is closer to 2/3. This difference is value is not surprising in light of the fact that within the quantum well the value of the quantum potential is not longer a correction. Indeed Q is approximately equal to the quasi-bound state energy.

The value of $\rho(x=0)$ from equation 16, with Q/3 replaced by 2Q/3 is:

(44) $\rho(Eq.(38)(x=0) = 5.043 \times 10^{16}/cm^3$

We note that the density upstream of the emitter is satisfactorily represented by equation (16). It would appear that our results are consistent with the discussion of Ancona and Iafrate (1989) where the quantum potential appearing in the moment equations should be

(45)   Phenomenological quantum potential: $aQ(x)$

where a is a position dependent positive constant less than unity.

The energy calculated from equation (18) with the center of the quantum well is

(46) $E_{cal}(x=0) = 2.864 \ mev/cm^3$

The energy calculated from equation (19) with Q/3 replaced by 2Q/3 is:

(47) $E_{Eq.(19)}(x=0) = 2.684 \ mev/cm^3$

The low value is present, even though the quantum potential tends to push up the mean carrier energy, and arises from the reduced charge in the quantum well.

CONCLUSION

This study represents the first comprehensive effort to assess through (1) numerical simulations of the equation of motion of the density matrix, and (2) approximate analytical procedures involving an expansion of the Liouville potential, the multiplicative constants associated with the quantum potential, as used in quantum hydrodynamic transport. It was found that when quantum effects are 'corrections' to classical calculations, as in $N^+N^-N^+$ structures the factor '1/3' is a satisfactory multiplicative constant. When the quantum potential is no longer a correction, as in the case of double barrier diodes, the multiplicative constant is no longer 'constant' but is position dependent and less than unity. Additional work is required to narrow the range of variation of this constant before effectively incorporating the quantum potential in detailed quantum hydrodynamic simulations of ultrasmall devices.

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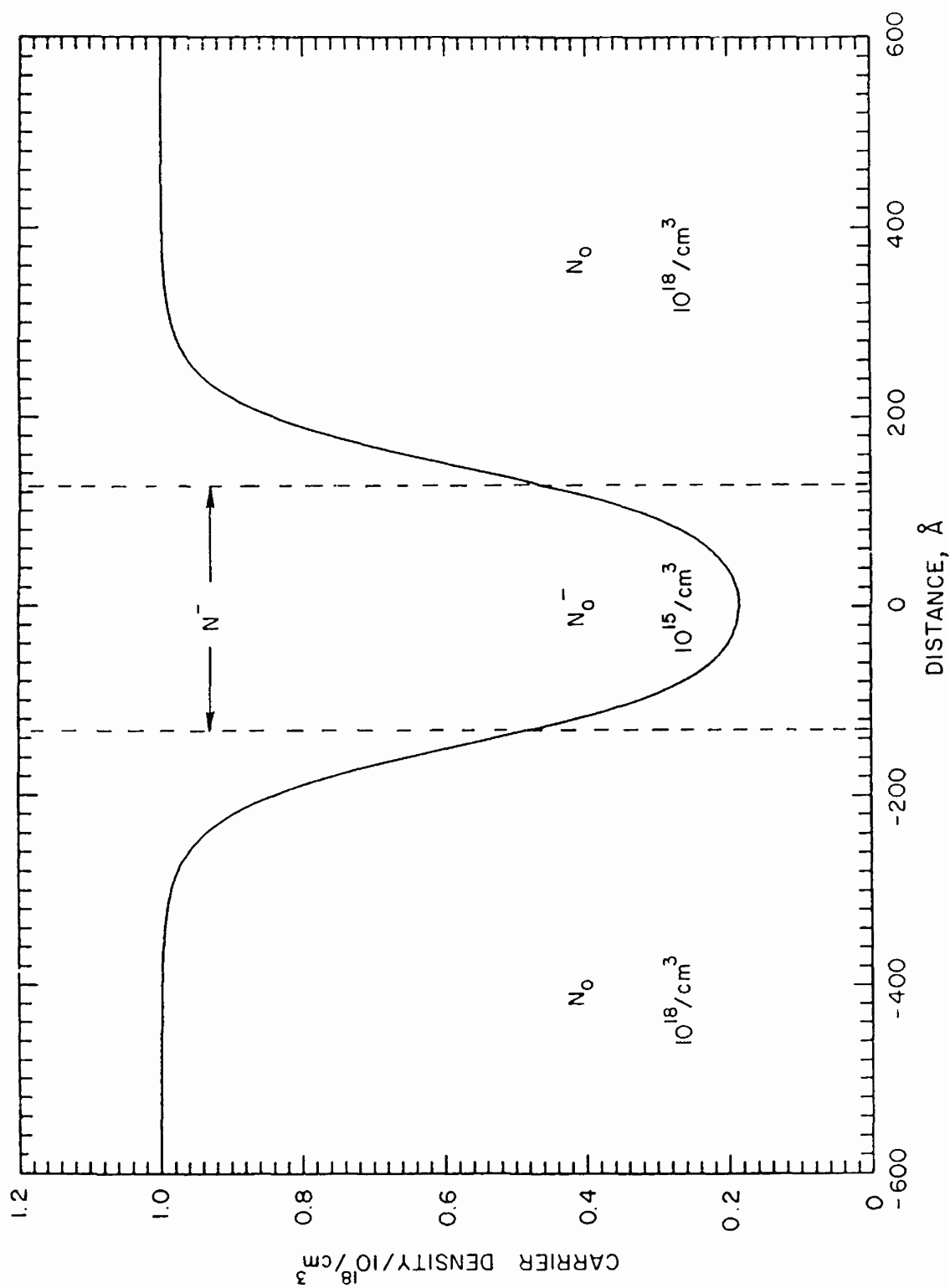
Fig. 1a. Carrier and background distribution for a NIN structure with free particle boundary conditions, as obtained from a solution of Equation (8) with zero dissipation and Poisson's Equation.
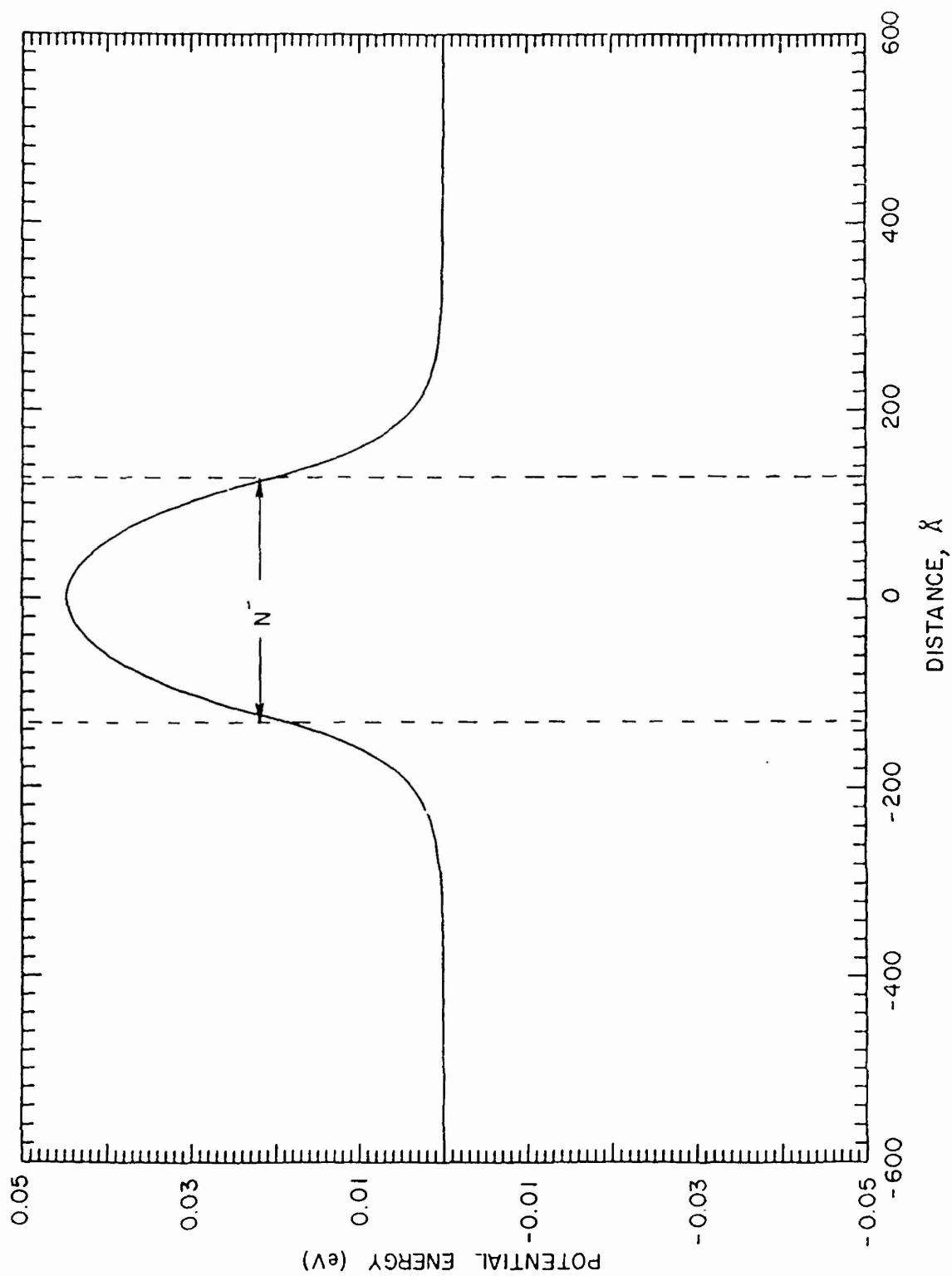
Fig. 1b. Self consistent potential associates with the density distribution of Figure 1a. The N^+N^- and N^-N^+ regions are indentified by the dashed lines.
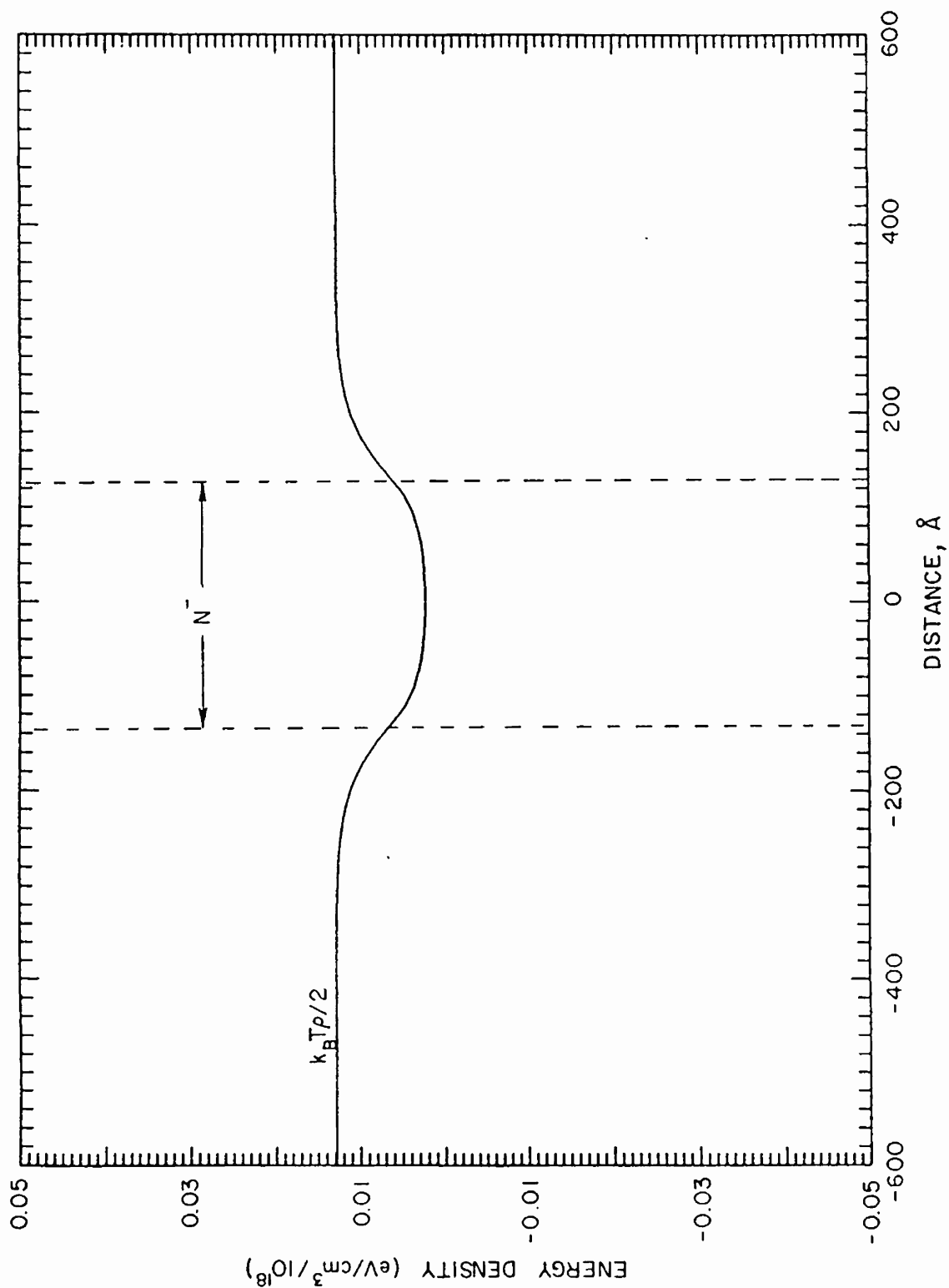
Fig. 1c. Energy density as obtained from Equation (18).
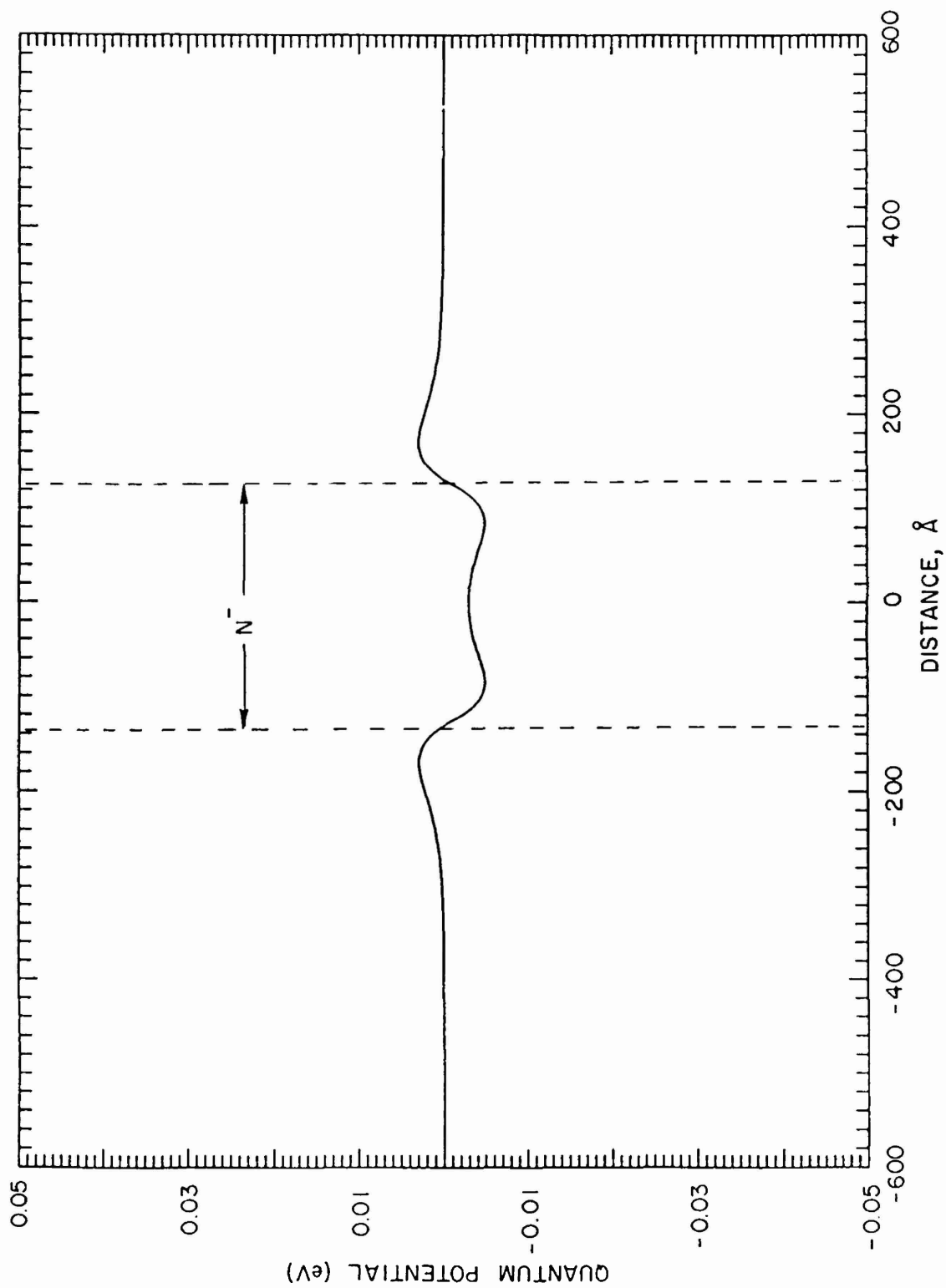Density at boundary region is entirely thermal.

Fig. 1d. Quantum potential for NIN structure, as obtained from Equation (1).

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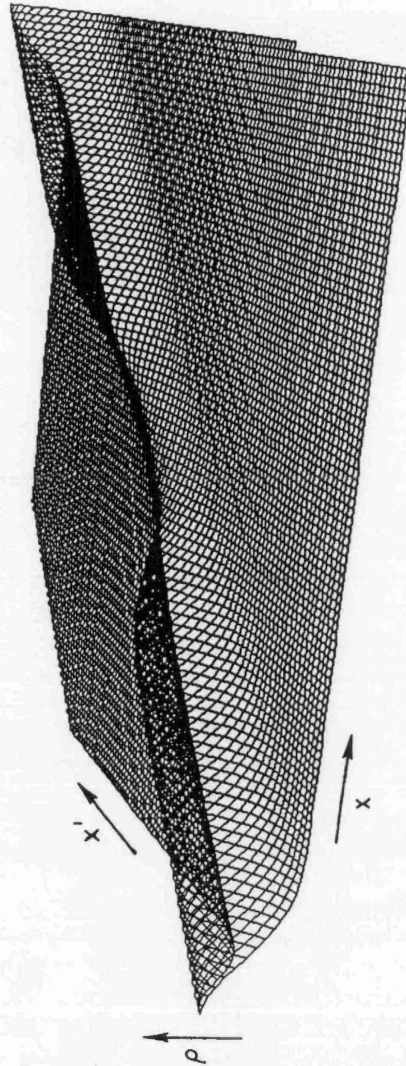
Fig. 2. Two dimensional representation of the density matrix, $\rho(x,x')$, for the NIN structure whose diagonal components are shown in Figure 1.
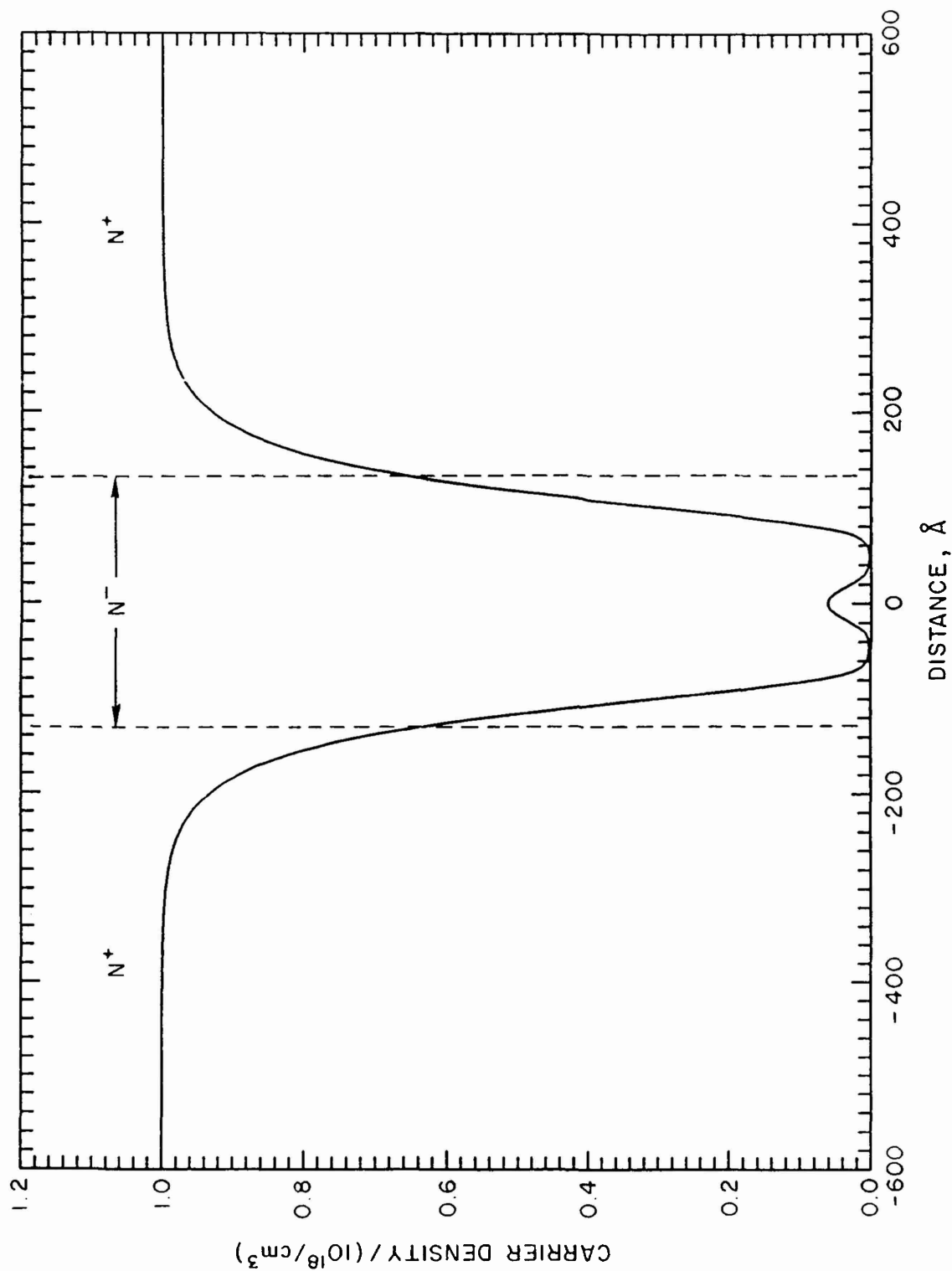
Fig. 3a. Carrier and background distribution for a $N^+N^-N^+$ structure with double barrier potentials in the N^- region. The barriers are each 30 meV high, 50 Å wide separated by a well that is 50 Å wide. The effective mass for this calculation is constant and equal to that of gallium arsenide. Free particle boundary conditions are assumed, and the equation of motion of the density matrix, Equation (8), is solved with zero dissipation, along with Poisson's equation.
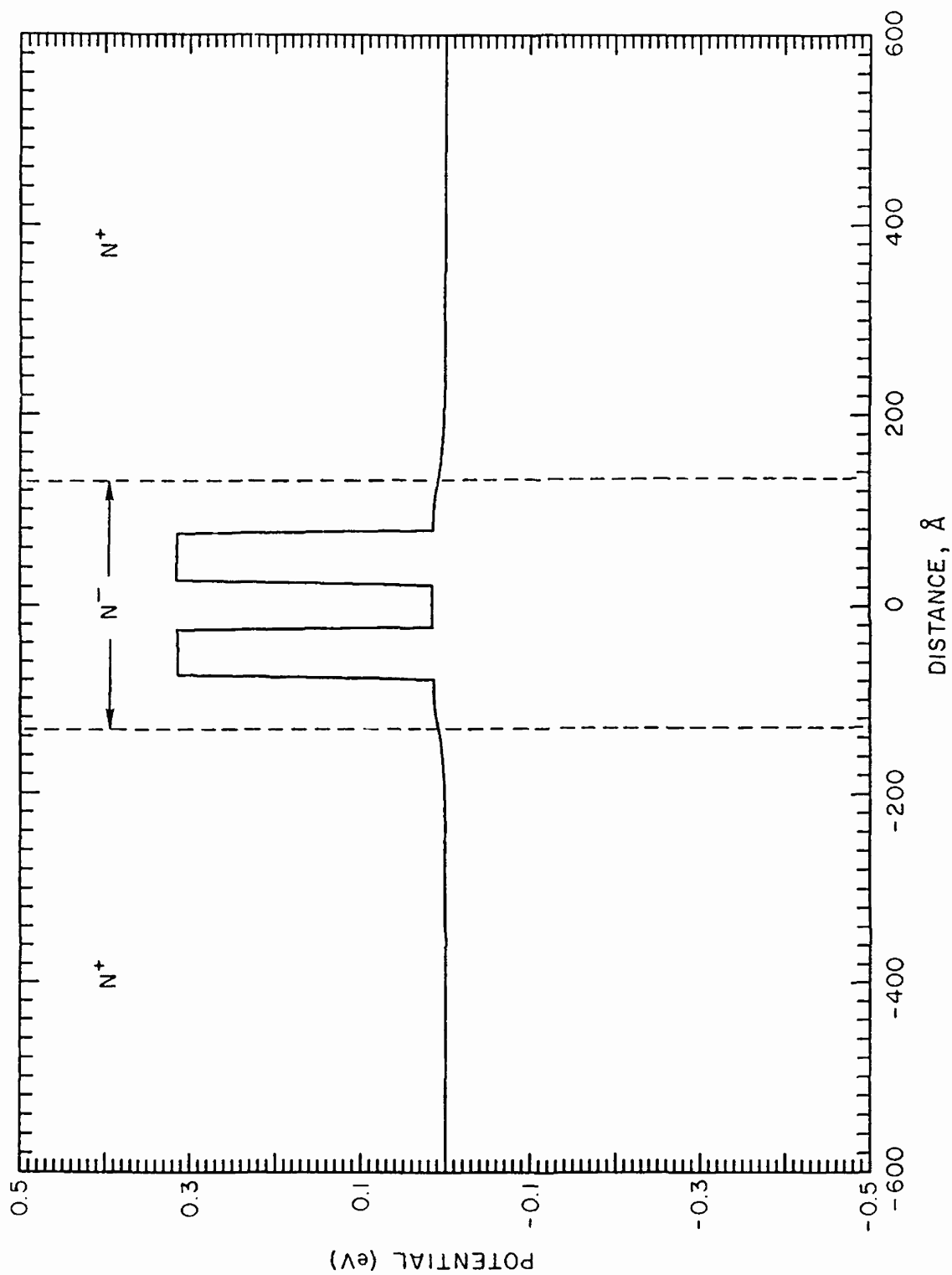
Fig. 3b. Self consistent potential plus heterostructure potential associated with the charge distribution of Figure 3a. The N^+N^- and N^-N^+ regions are identified by the dashed lines.
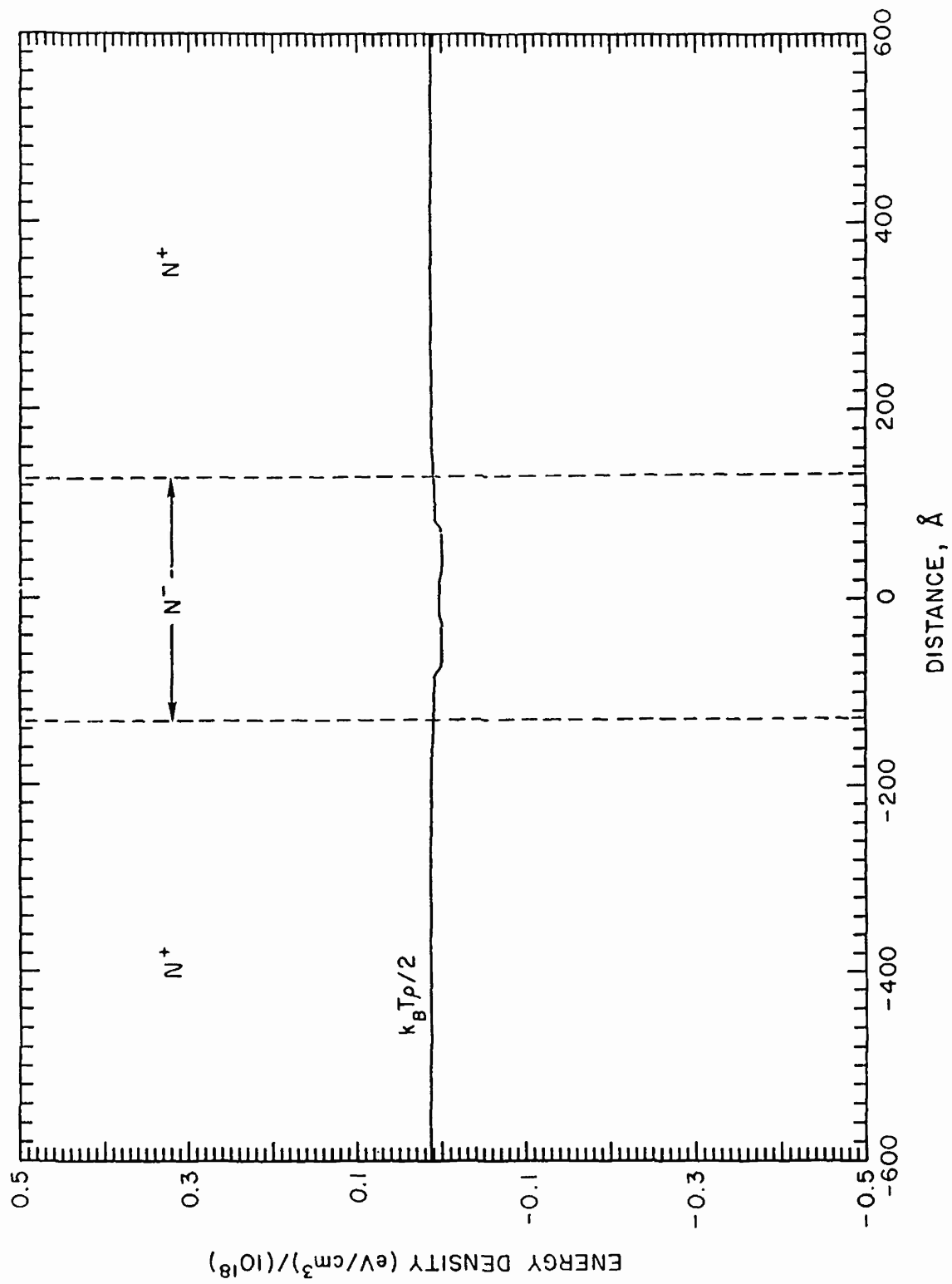
Fig. 3c. Energy density as obtained from Eq. (18). Energy density at boundary region is entirely thermal.
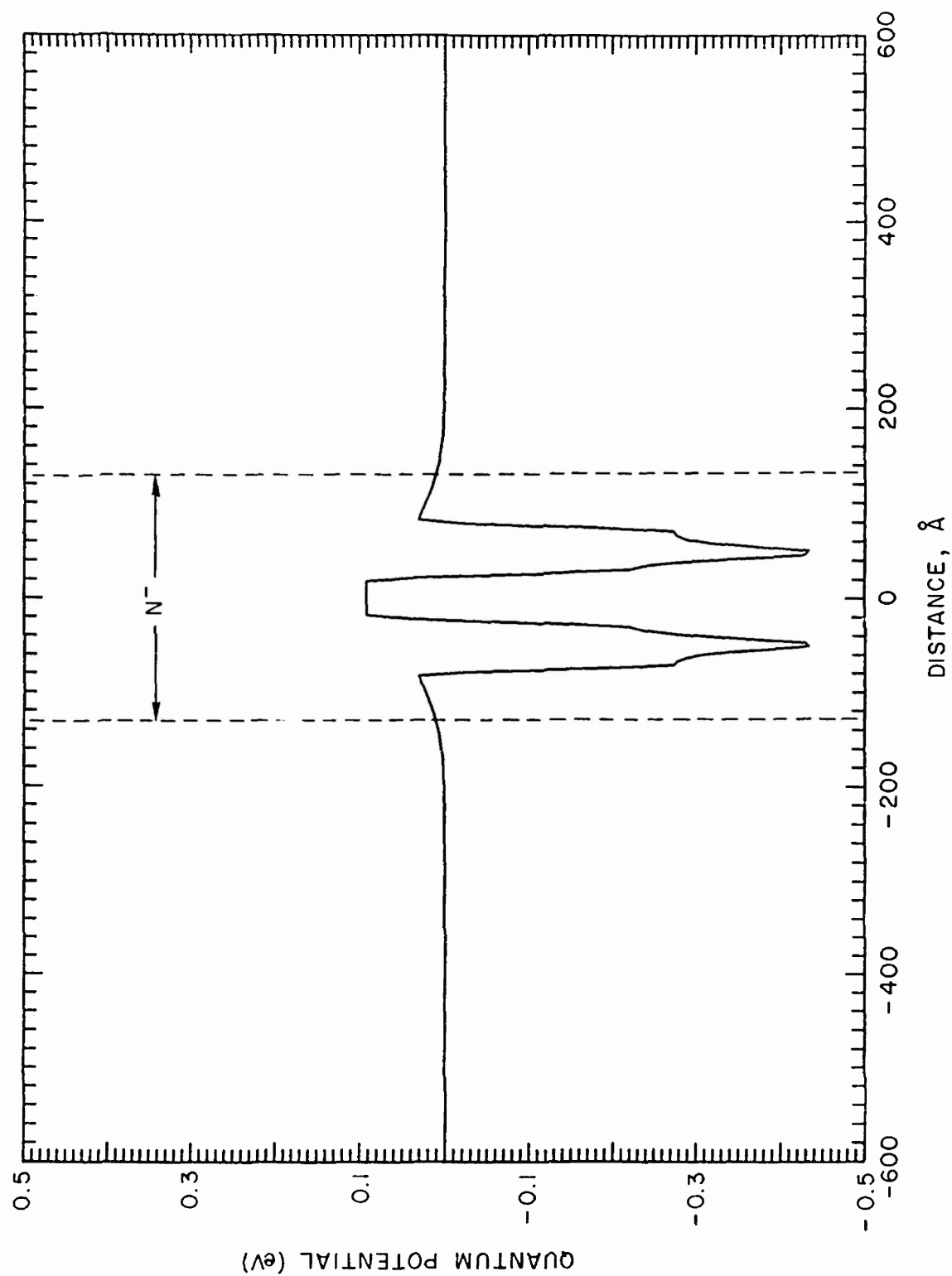
Fig. 3d. Quantum potential for the charge distribution of Figure 3a as obtained from Equation (1).
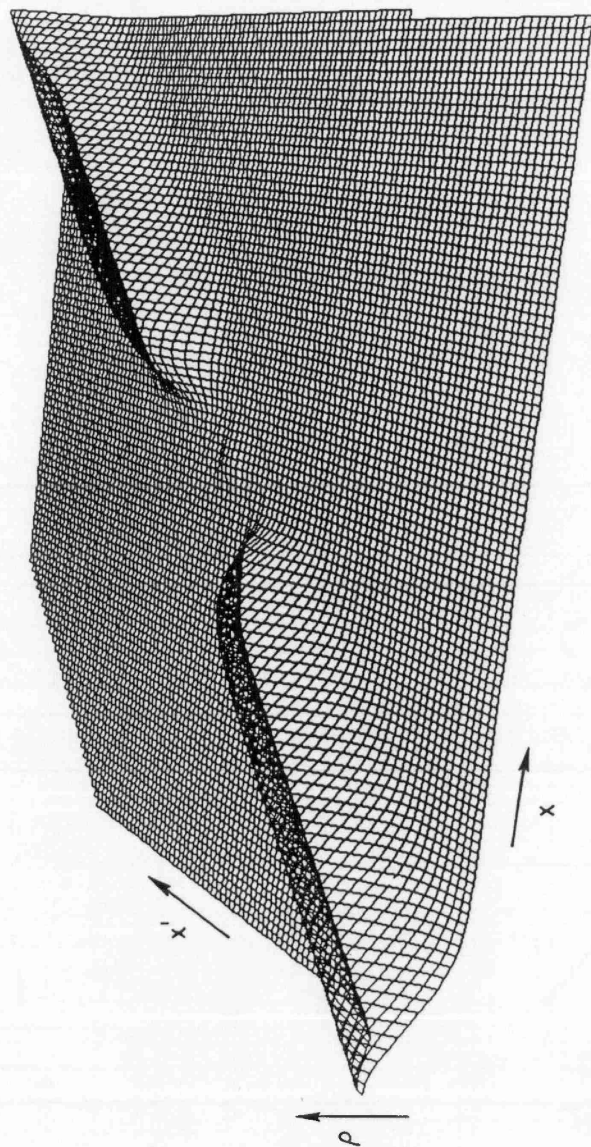
Fig. 4. Two dimensional representation of the density matrix, $\rho(x,x')$, for the double barrier structure whose diagonal components are shown in Figure 3.